

Chloral

75-87-6 | DTXSID7024744

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.54×10^{-1} mol/L

Global applicability domain: Inside

Local applicability domain index: 7.26×10^{-1}

Confidence level: 5.52×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Chloral

Measured: 2.04×10^{-1}

Predicted: 1.54×10^{-1}

Image not found

2-Chloroethyl vinyl ether

Measured: 4.03×10^{-3}

Predicted: 3.06×10^{-2}

Image not found

2,4-Pentadienenitrile

Measured: 1.90×10^{-1}

Predicted: 2.46×10^{-1}

Image not found

Epichlorohydrin

Measured: 7.12×10^{-1}

Predicted: 8.45×10^{-1}